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DIFFICULTY AND POSSIBILITY OF KINETIC THEORY OF QUANTUM-MECHANICAL SYSTEMS

Part VI - Summary, Addenda and Conclusion

by

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TABLE OF CONTENTS

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SUMMARY

This part concludes the series of the reports written thus far under the same title. The conclusion is that quantum-mechanical states are of ensembles. The notion of ensemble is exactly one hundred years old. It was first conceived by Boltzmann in 1871. In this century, the notion has been somehow distorted. The genuine notion has survived barely as anomalous and obscure. This part is a tribute to those anomalous authors who have fought, with no concent of the majority, for the survival of the true notion of ensemble. The author now believes that the point of departure for truely effective physics should be found by recognizing the old notion of ensemble, its merit and the limitation.

I. INTRODUCTION

In classical mechanics, we always assume that a complete description of the state of a physical system is possible in principle. If we cannot measure and calculate completely and precisely those variables and their dynamical relations, yet we assume that they exist. In classical kinetic theory, our main task is to derive coarse-grained variables and their relations from the precise description of a system. In this sense, classical kinetic theory is a deductive method. In quantum mechanics such a description of a system is impossible. As a simple example, the position vector and the momentum of a single particle cannot exist simultaneously. Suppose that by an experimental method we have known that electrons are distributed nonuniformly in a domain of space. According to this information, we give the description of the electrons as precisely as possible in terms of plane de Broglie waves. The Fourier expansion is made with respect to momentum variables so that the spatial nonuniformity is represented. By the conventional method, we then quantize the field. The spatial nonuniformity of the distribution is now converted to a non-uniform momentum distribution of quantized electrons. Is this information enough for treating kinetic-theoretical phenomena

which really take place in the system, being supposed to be quantum-mechanical?

In Part I of this report, it was demonstrated that Pauli's exclusion principle should be applied only in a narrow domain of space. In Part II, the Schrodinger equation is transformed to the quantum-mechanical Liouville equation, and conventional quantum-mechancial states are shown to be of stationary ensembles. In Parts III and IV, conventional Hamiltonian matrices of electron-electron and electron-photon interactions are shown to involve significant and unremovable effects of the scale of space chosen arbitrarily for quantization of concerned fields; the situation is readily expected by the ensemble interpretation of wave functions. It is noted that those interactions are kinetic-theoretical, and should be out of the scope of conventional quantum mechanics. In Part V, particular and general solutions of the Schrodinger equation are given. One of the particular solutions is a stable wavelet. It is shown that a de Broglie wave is constructed with many similar wavelets. Furthermore a wavelet turns out to be the known δ-function representation of a classical material point in the phase space at a certain limit. This wavelet bears an information of particle which is necessary for treating kinetic-theoretical phenomena and is

missing in a de Broglie wave. We recall, it was shown, as of appendix of Part I, that the Dirac equation, and hence the Schrodinger equation, and the Maxwell-Lorentz equations are derivable by linearizing a set of covariant tensor equations for a non-Euclidean field. The wavelet seems to be the simplest and closed model of the field.

In this report, the last part of the same series, it is first pointed out that the notion of ensemble and its limited role in kinetic theory were first introduced by Boltzmann and then by Maxwell a century ago. In this century since Gibbs, its original meaning has become obscure. Only as an anomalous and vague opinion, it has barely survived. The historical circumstances are outlined in section II and section III. It is emphasized that the merit of Gibbs's statistical mechanics and quantum mechanics should never be minimized by this study. Only what is said is that we have to recognize the limitation of their validity, as we should expect of any doctrine of science. The distorted notion of ensemble has caused similar difficulties in various fields of modern physics; for example, we may also mention turbulence theory in fluid mechanics. In general, <u>the same difficulty is found unmistakably in any place where elementary processes are nonlinear</u>.

II. GIBBS'S ENSEMBLE

In statistical mechanics initiated by Gibbs(ref.1), the concept of ensemble of similar systems is indispensable. Therefore we sometimes think that the concept was also made by Gibbs. This is false in one sense, and true in the other.

As is pointed out by Gibbs himself, the explicit consideration of a great number of similar systems and their distribution in phase is perhaps first found in one of Boltzmann's papers published in 1871. Maxwell in 1879 (ref.2) also writes in his paper "On Boltzmann's Theorem on the Average Distribution of Energy in a System of Material Points" as follows:

"The only assumption which is necessary for the direct proof is that the system, if left to itself in its actual state of motion, will, sooner or later, pass through every phase which is consistent with the equation of energy."

"I have found it convenient, instead of considering one system of material particles, to consider a large number of systems similar to each other in all aspects except in the initial circumstances of the motion, which are supposed to vary from system to system, the total energy being the same in all. In the statistical investigation of the motion, we confine our attention to the number of these systems which at a given time are in a phase such that the variables which define it lie within

given limits...

If the number of systems which are in a given phase (defined with respect to configuration and velocity) does not vary with time, the distribution of the systems is said to be steady."

Subsequently, Maxwell concludes that there must be the constancy of a function of variables, if not the only solution, of the problem of a steady distribution, in accordance with the energy conservation law.

If one reads Gibbs's statistical mechanics (ref.1), on keeping in mind those statements given by Maxwell and the content of Maxwell's distribution function which is the representation of canonical ensemble of particles, one might wonder what is new there. In fact, however, there is a significant difference between Maxwell-Boltzmann's gas theory and Gibbs's statistical mechanics, as is summarised in the following:

The ideal of Maxwell and Boltzmann was that all about gas theory should turn out theorems derivable from Newton's equations of motion governing precisely an enormous number of corpuscles which they believe to constitute a gas. Therefore, consideration of ensemble is merely a mathematical convenience of treating a many-particle system under the special condition that the gross state of a gas is stationary or in equilibrium. On the other hand, Gibbs was more ambitious: He intended to derive the ultimate law of thermodynamics, not only of gases but of systems in any state,

from rational mechanics of systems under consideration. For doing so, Gibbs took Maxwell-Boltzmann's gas theory merely as a suggestion of the possibility of his approach, and abandoned the hypothesis of corpuscles, which was as yet ambiguous at the time and also too difficult to maintain in treating systems in liquid and solid states. He assumed that a system has a large number of degrees of freedom, but is not necessarily constituted of discrete corpuscles. He states:

"... Even if we confine our attention to the phenomena distinctively thermodynamics, we do not escape difficulties in as simple a matter as the number of degrees of freedom of a diatomic gas. It is well-known that while theory would assign to the gas six degrees of freedom per molecule, in our experiments on specific heat we cannot account for more than five. Certainly, one is building on an insecure foundation, who rests his work on hypothesis concerning the constitution of matter.*

Difficulties of this kind have deterred the author from attempting to explain the mysteries of nature, and have forced him to be contented with the more modest aim of deducing some

*This difficulty was solved ten years later by Einstein, Ehrenfest and others, not by abandoning the corpuscle hypothesis but by considering the quantum-theoretical characteristic of a corpuscle.

of the more obvious propositions relating to the statistical branch of mechanics. Here, there can be no mistake in regard to the agreement of the hypothesis with the facts of nature, for nothing is assumed in this respect. The only error into which one can fall, is the want of agreement between the premises and the conclusion, and this, with care, one may hope, in the main, to avoid."

By this approach, Gibbs's statistical mechanics transcends gas theory and is useful for treating systems not only in gaseous state but also in liquid and solid states. This is a great merit of Gibbs's statistical mechanics. At the same time, however, Gibbs made a rather careless statement (ref. 1, p.141):

"An ensemble of systems distributed in phase is a less simple and elementary conception than a single system. But by the consideration of suitable ensembles instead of single systems, we may get rid of the inconvenience of having to consider exceptions formed by particular cases of the integral equations of motion, these cases simply disappearing when the ensemble is substituted for the single system as a subject of study. This is especially true when the ensemble is distributed, as in the case called canonical, throughout an extension-in-phase. In a less degree it is true of the microcanonical ensemble, which does not occupy any extension-in-phase, (in the sense in which we have used the

term,) although it is convenient to regard it as a limiting case with respect to ensemble which do, as we thus gain for the subject some part of the analytical simplicity which belongs to the theory of ensembles which occupy true-extension-in-phase."

As Maxwell stated explicitly in 1879, the notion of ensemble is conveninet and useful when one treats a system in equilibrium. In the above statement, however, Gibbs does not emphasize this condition. The following success of Gibbs's statistical mechanics has led people to tend to believe that Gibbs's statistical view or representation of a system is universally valid. Later in 1938, Tolman* states (ref.3, p.69):

"Impressed by the exact character of the principles of classical mechanics, and also by the actual regularities in the macroscopic behavior of systems composed of many molecules, they apparently hoped to secure really precise results for such systems by the temporary introduction of an hypothesis which might itself be validated from principles of mechanics proper, and did not sufficiently appreciate that a further essentially statistical assumption would be needed even if their hypothesis were valid."

---

*In this quotation, they mean Maxwell, Boltzmann, and others who advocated the corpuscle hypothesis. Tolman also adds as of footnote as follows: "This failure to adopt a truely statistical viewpoint is not to be ascribed to Gibbs."

Such being the general trend, it was natural that Yvon(1935), Bogoliubov(1946), Born and Green(1946), and Kirkwood(1946) independently advanced similar approaches of kinetic theory, beginning with the Liouville equation, by assuming that a system should belong to Gibbs's canonical ensemble. Unlike in statistical mechanics, a system treated in kinetic theory is not in thermal equilibrium. The system evolves due to correlative and stochastic processes taking place in the system. Those processes are governed by non-linear equations, and the integrals of motion of the entire system are not sufficient for describing the system; local densities of energy, of momentum and of mass are necessary for representing the dynamical characteristics of the system. A particle in a system represented by an ensemble does not exist in any definite state. It exists in all the possible states, as many as the number of points considered in the concerned domain of the phase space. Therefore, there is no consistent way of considering microscopic and correlative behaviors of particles. It is possible to say that kinetic theories developed since Gibbs have all suffered from similar difficulties, as has been discussed in detail by the author (ref.4).*

*Earlier ter Haar suggested the possibility of the same difficulty (ref. 5). If the deviation of the state of a system from thermal equilibrium is slight, it is possible to linearize the macroscopic effect so that some assumed coefficients may represent the effect, as shown by Onsager (ref. 6).

III. QUANTUM-MECHANICAL STATES

Schrodinger(1926) showed that by considering the whole series of eigen-states of a system governed by the Schrodinger equation one may derive axioms and principles of quantum mechanics as theorems. Schrodinger seemed to imply that a wave function is a realistic description of some physical field. But in quantum mechanics, a wave function is the ultimate representation of a physical system, in the same way as Gibbs's ensemble is the complete representation of a physical system in statistical mechanics. There is no more detailed information.

However, some authors have expressed some suspicion as regards the completeness of quantum mechanics as a system of physical laws, particularly when quantum mechanics claims that the ultimate human knowledge of nature is provided and limited by quantum-mechanical principles. The discontinuity of reasoning and knowledge required by quantum mechanics, such as seen in acausal jump and particle-wave dualism, causes in some minds an intolerable uneasiness or even pain, as was expressed earlier by Margenau (ref.7).

According to de Broglie (ref.8), his interpretation that the significance of the de Broglie wave is not in the wave itself but in its phase, is almost as old as the wave itself:

The propagation of a wave is not the description of the physical reality of a particle. The direct description of a particle is the u wave which has the same phase as the de Broglie wave and is localized in space. A localized wave, as a description of a particle, is more informative than a plane wave. In recent years, three anomalous theories are known:

Wiener and Siegel show, by employing a statistical approach developed for Brownian motion (ref.9), how ensemble of completely described systems obeying a postulated dynamics can be so constructed as to have the same statistical properties that are expressed by a given quantum-mechanical function.

Bohm (ref.10) postulates that a particle is always accompanied by field ψ. Between them, there is a sort of quantum force. Because of sub-quantum states which are not completely described by quantum mechanics, the state of a particle interacting with the accompanying field is fluctuating, like a particle undergoes the Brownian motion in a medium. On this postulation, Bohm claims, all the quantum-mechanical phenomena can be explained without employing such principles as dualism, acausal jump, etc. The conventional theory of interference of electron with itself is also replaced with an explanation as based on quantum force.

Landé (ref.11) also intends to eliminate the strong discontinuity of reasoning in quantum mechanics. He first puts

three quantum rules: 1)Planck's energy quantum rule; 2) Sommerfeld-Wilson's angular-momentum quantum rule; 3) Duane's linear-momentum quantum rule (ref. 12). The third rule distinguishes remarkably Landé's interpretation from the others. He also claims that there are neither continuous matter waves filling the whole space nor discontinuous photon dashing about. As regards wave functions, he writes:

"A ψ-function is a well-ordered list of betting odds, based on statistical experience, for the diverse outcomes of specific tests of a microscopic object with a macroscopic instrument."

" ψ-functions are tables of probabilities for events."

Besides those interpretations, there are criticisms of quantum mechanics. Bohm (ref.13) and Bell (ref.14) showed that von Neumann's proof that quantum mechanics does not permit a hidden-variable interpretation is not so complete as it appeared earlier. Recently Margenau (ref.15) demonstrated that the validity of the exclusion principle is conditional, as depending on spatial coordinates which are significant in physical reality but are ignored in conventional quantum mechanics.* This demonstration implies the necessity of modification of the concept of indistinguishability of similar particles. It also implies

*A similar demonstration was also made in Part I of this report.

the necessity of modification of the concept of measurement in quantum mechanics, if quantum mechanics intends to meet experimental realities.

Those anomalous interpretations and criticisms are different one after another. But there is one notion which is shared commonly by them: The role assigned to wave functions by those authors is much similar to the role of ensemble, as representing a single system, conceived by Boltzmann, Maxwell and Gibbs.* However, they have failed thus far to demonstrate the indispensability of this notion in the truely physical sense. In fact, therefore, most of the contemporary physicists tend to think that orthodox quantum mechanics is as yet intact and is not necessary to be changed, at least in the pragmatical sense. As we have seen in this report, those anomalous interpretations published earlier seem to contain some truth.

*Bohm's quantum force does not completely fit the ordinary concept of ensemble. Obviously Lande does not like his theory to be so specific as regarded ensemble theory. If the difference among those authors is emphasized: 1) Landé does not intend to modify the conventional formalism of quantum mechanics; he only intends to eliminate the strong discontinuity of reasoning; 2) Wiener and Bohm explicitly, and Margenau and Bell tacitly make some predictions about transient phenomena which quantum mechanics may fail to treat.

IV. DIFFRACTION OF ELECTRONS

Davisson and Kunsman in 1923, and Davisson and Germer more in detail in 1927, found the diffraction phenomenon of electrons scattered on surfaces of crystals. There were two ways of explanation. One was made by Einstein on assuming that electrons are represented by de Broglie's matter waves. The other by Duane on assuming the existence of linear-momentum quantum. William Duane's paper entitled "The Transfer in Quanta of Radiation Momentum to Matter", primarily dealing with X-ray diffraction, was published in Proceeding of National Academy of Science(U.S.A.), Vol.9, pp.158-164, 1923, being communicated on March 2, 1923. It is said the date is a few months ealier than de Broglie's proposal of matter waves.

As regards Duane's theory, Born and Biem (ref.16) write: "Every physicist must accept Duane's rule, which describes correctly all experiments of momentum exchange on periodic structures. But he has learned little if he accepts it. On the other hand, de Broglie's paper of September 1923 contains the beginning of an insight. In this work Planck's and Duane's rules were connected. Using the theory of relativity, de Broglie associates with the four-vector of momentum and energy the four-vector of wave number and frequency..." Since Born was one of the most faithful advocators of orthodox quantum mechanics, this remark

made by him on Duane's theory is impressive. If we accept Duane's explanation, as Lande does, it is easy to interpret quantum-mechanical states as of ensembles. If not, it is fairly difficult to put ensemble interpretation of quantum-mechanical states and electron diffraction in harmony. Landé took the easy way; Wiener and Bohm chose the hard way. (The meaning of ensemble given by Bohm and Wiener is not the same as of Boltzmann, Maxwell and Gibbs; in the former a system of an ensemble is not completely independent of the others.) All of our discussions, in this series of reports, have been made by assuming tacitly the existence of Duane's explanation. The author believes, particularly after the study given in Part V of this report, Duane's theory is indispensable.

The history of physics is not straightforward. If Einstein had not given the explanation of electron diffraction by employing de Broglie's matter waves in 1924 and 1925, Schrodinger probably would not have made his wave mechanics in 1926. But now, by ana ing the Schrodinger equation, we are obliged to choose Duane's theory. By reading carefully de Broglie (ref.8) and Bohm(ref.10), it is my impression that, if they had abandoned Einstein's theory of electron diffraction earlier, they would have reached a clear interpretation of quantum mechanics as they intended at the beginning. By so doing, the merit of the de Broglie wave would never be minimized.

V. CONCLUSION

A particle governed by the Schrodinger equation is neither material point nor continuous wave. As was conceived by Einstein in 1919, it must be a sort of fieldlet (Supplement to Part I, and Part V). Quantum-mechanical states are of ensembles (Part II and Part V). This view may unify those pioneering and anomalous views advanced by various authors (Part VI). By this view, we may avoid difficulties of conventional quantum mechanics, dealing with stochastic processes of interactions among particles (Part III and Part IV).

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Part II - The Quantum-mechanical Liouville equation and its Solutions: PIBAL Report No. 70-26, May 1970.

Part III - Inconsistent Scale Effects in the Theory of Scattering: PIBAL Report No. 70-35, July 1970.

Part IV - Inconsistencies in Representation of Photon-Electron Interaction: PIBAL Report No. 70-35, July 1970.

Part V - Particular and General Solutions of the Schrodinger Equation and their Significance in Kinetic Theory: PIBAL Report No. 70-36, Aug. 1970.

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13. ABSTRACT

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